

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
 Data File : BG029312.D
 Acq On : 17 Oct 2017 22:11
 Operator : SJ/JU
 Sample : I5817-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TANK-3

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.245	325	333	342	rBV	59943	95055	1.59%	0.364%
2	5.720	407	414	426	rBV	422756	687500	11.49%	2.632%
3	7.319	679	686	696	rBV	278862	500301	8.36%	1.915%
4	7.700	743	751	761	rBV	824251	1412123	23.60%	5.406%
5	8.171	823	831	838	rBV	255543	449667	7.51%	1.721%
6	8.494	878	886	899	rBV	1072153	1880089	31.42%	7.198%
7	9.334	1019	1029	1041	rBV	935826	1688255	28.21%	6.463%
8	10.985	1302	1310	1319	rVB	410727	746686	12.48%	2.859%
9	13.417	1716	1724	1738	rBV	2756689	4391013	73.38%	16.810%
10	14.228	1856	1862	1867	rBV	48240	69102	1.15%	0.265%
11	14.786	1950	1957	1968	rBV2	701873	1118867	18.70%	4.283%
12	16.267	2198	2209	2223	rBV	1503652	2338749	39.09%	8.953%
13	17.524	2416	2423	2435	rBV2	892092	1376536	23.00%	5.270%
14	18.394	2566	2571	2581	rBV	84231	139986	2.34%	0.536%
15	19.651	2781	2785	2795	rBV	127375	195931	3.27%	0.750%
16	20.115	2858	2864	2877	rBV	4504513	5983688	100.00%	22.907%
17	21.796	3143	3150	3161	rVB	908607	1528776	25.55%	5.853%
18	25.104	3702	3713	3731	rBV3	490421	1518778	25.38%	5.814%

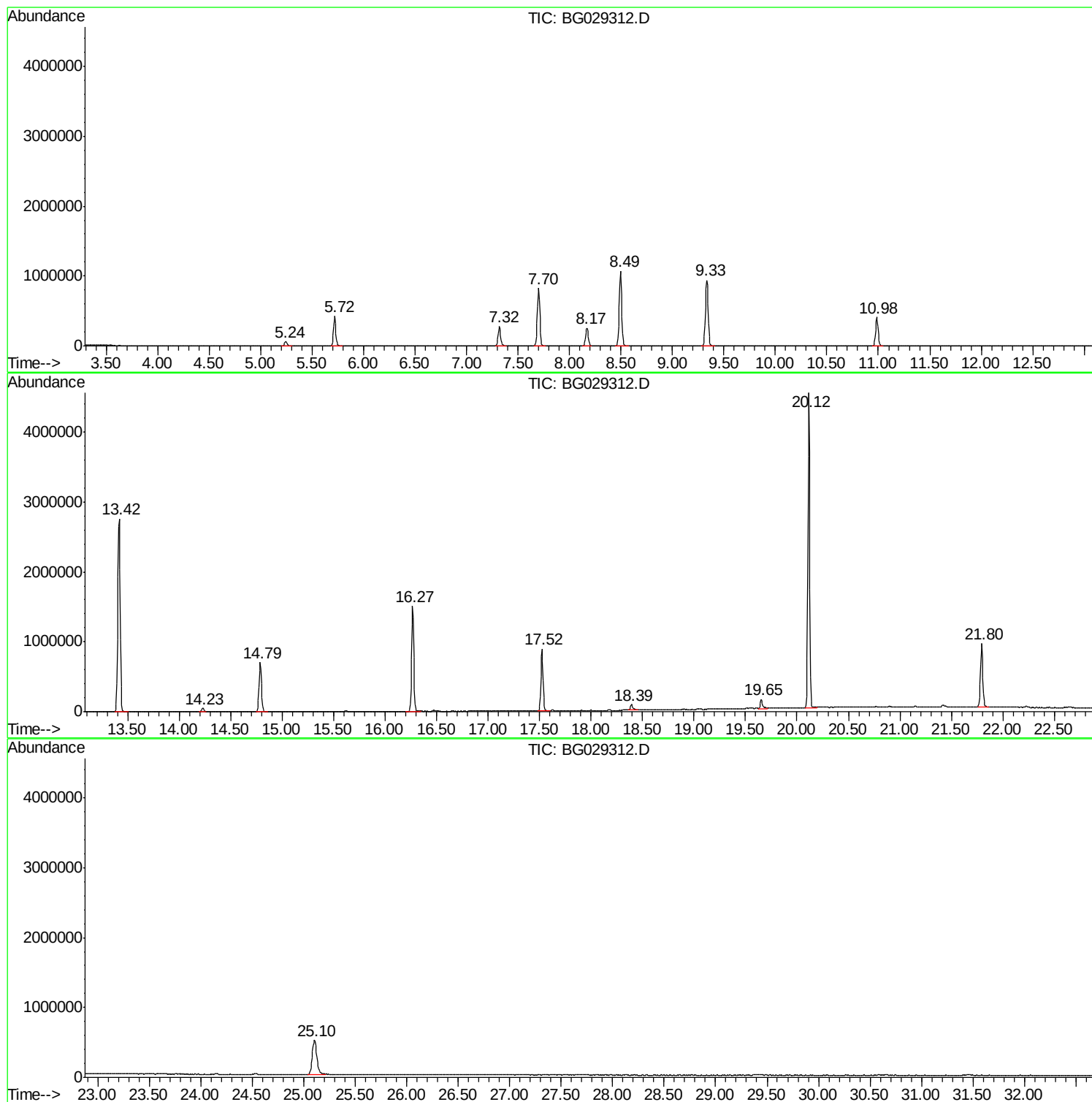
Sum of corrected areas: 26121102

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029312.D
Acq On : 17 Oct 2017 22:11
Operator : SJ/JU
Sample : I5817-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-3

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029312.D
Acq On : 17 Oct 2017 22:11
Operator : SJ/JU
Sample : I5817-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-3

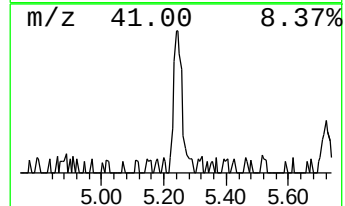
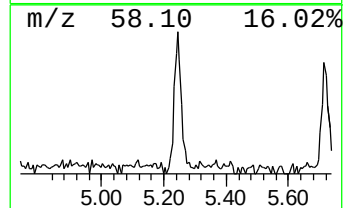
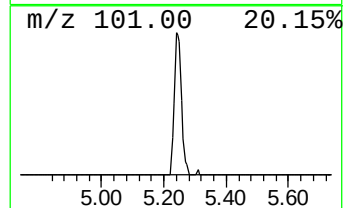
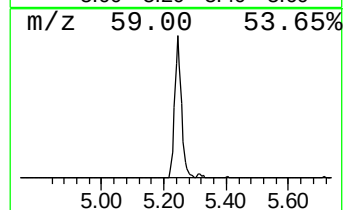
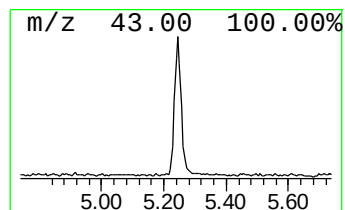
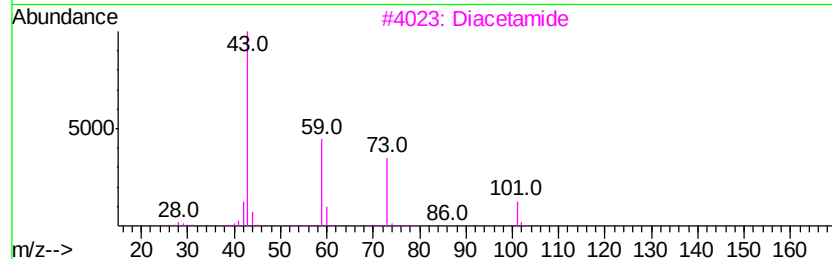
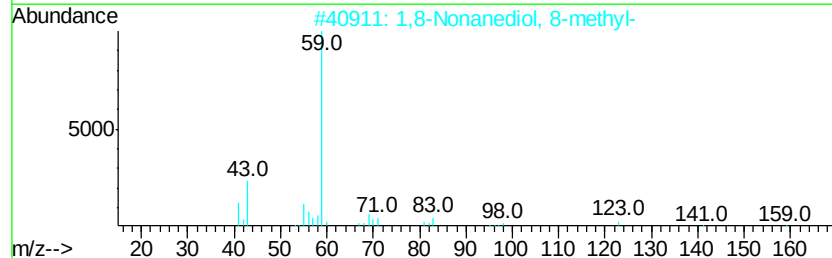
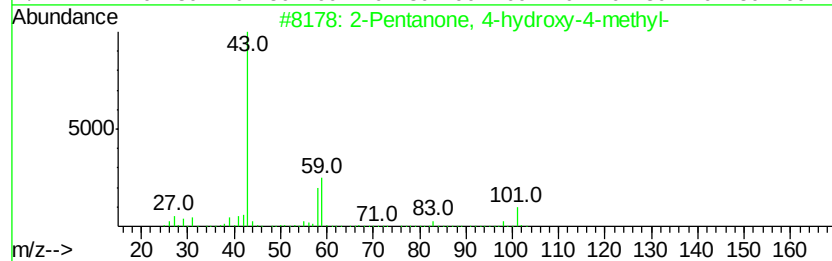
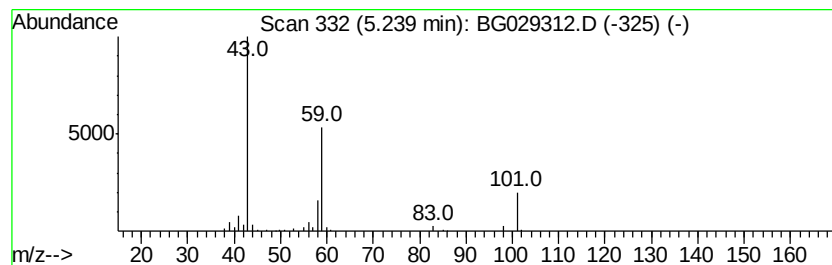
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	4.23 ng	95055	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3		Diacetamide	101	C4H7NO2	000625-77-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029312.D
Acq On : 17 Oct 2017 22:11
Operator : SJ/JU
Sample : I5817-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-3

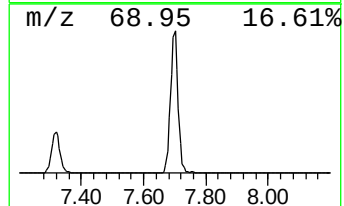
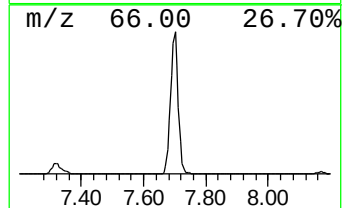
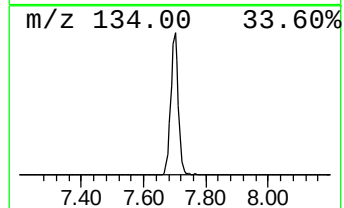
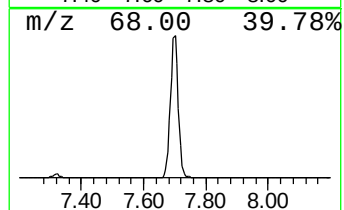
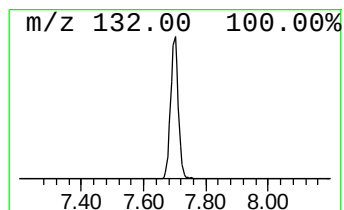
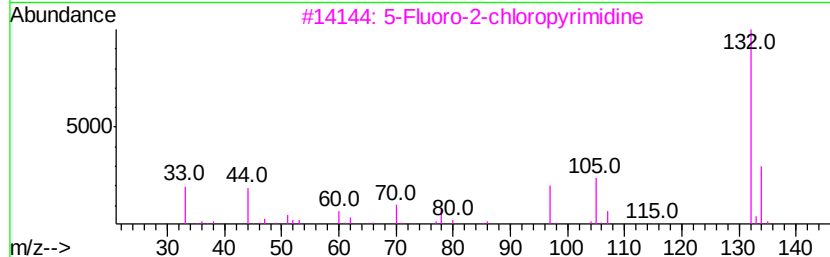
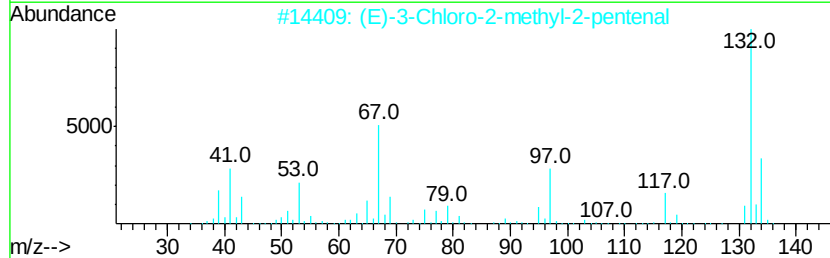
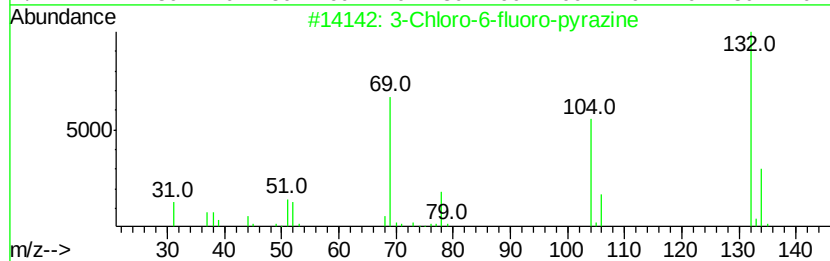
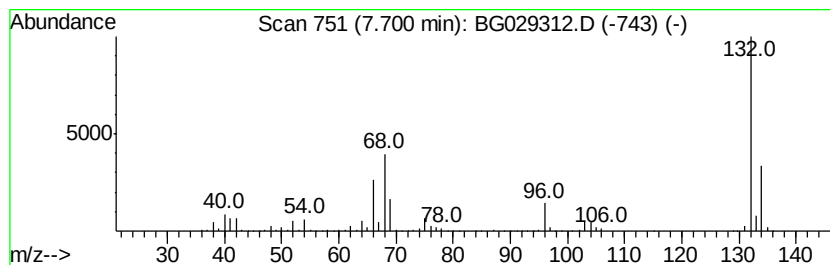
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	62.81 ng	1412120	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029312.D
Acq On : 17 Oct 2017 22:11
Operator : SJ/JU
Sample : I5817-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-3

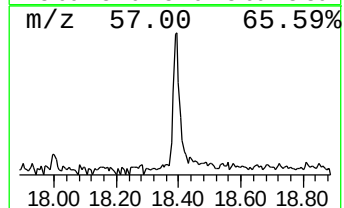
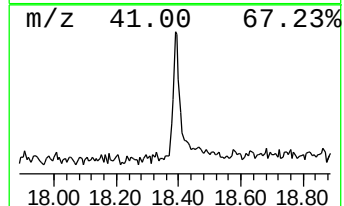
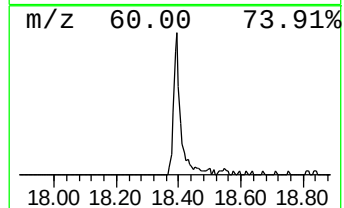
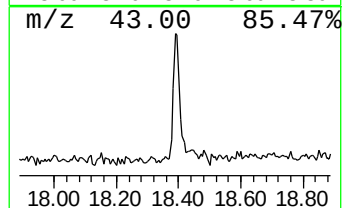
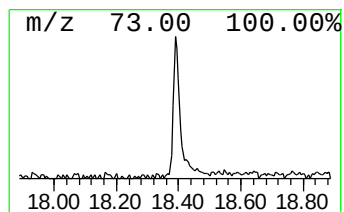
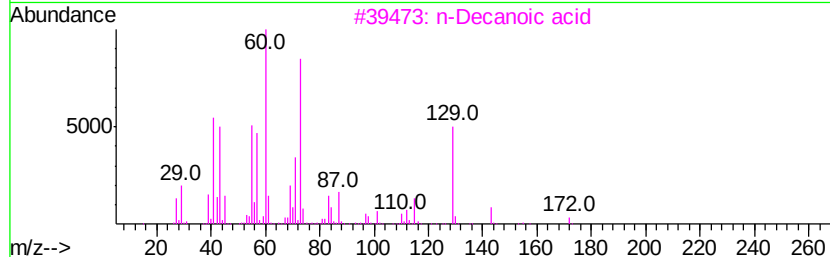
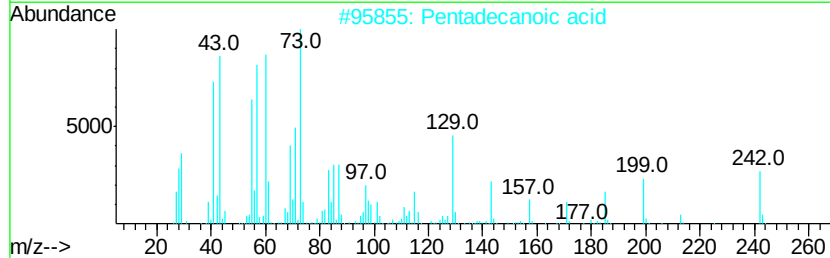
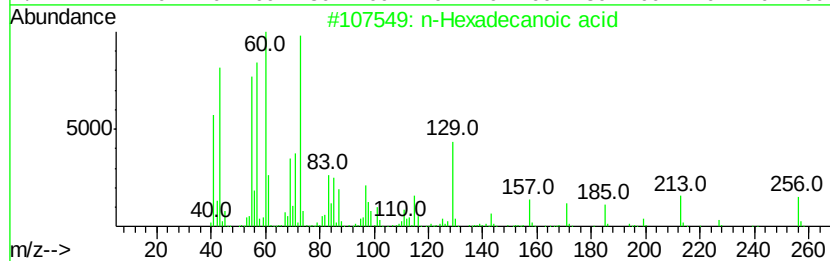
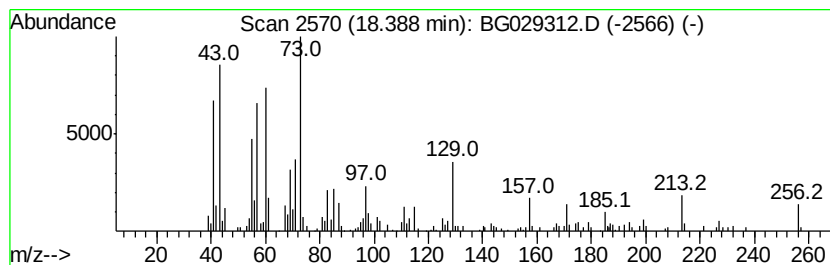
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.03 ng	139986	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	n-Decanoic acid	172	C10H20O2	000334-48-5	78
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029312.D
Acq On : 17 Oct 2017 22:11
Operator : SJ/JU
Sample : I5817-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-3

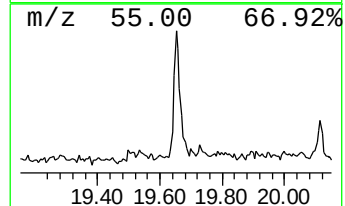
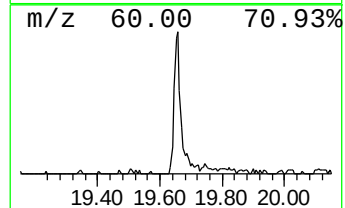
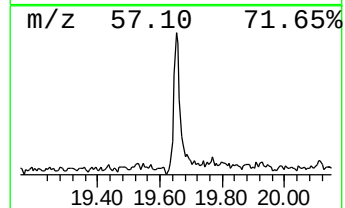
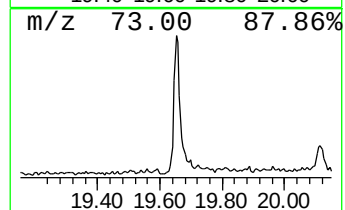
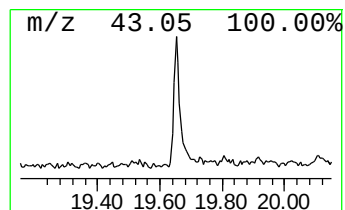
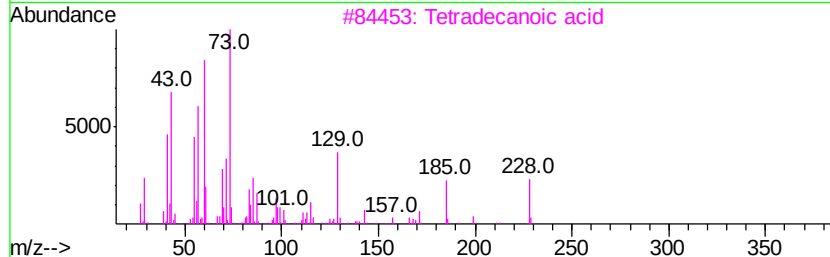
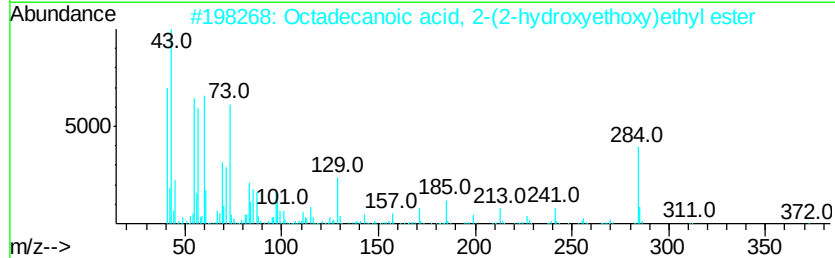
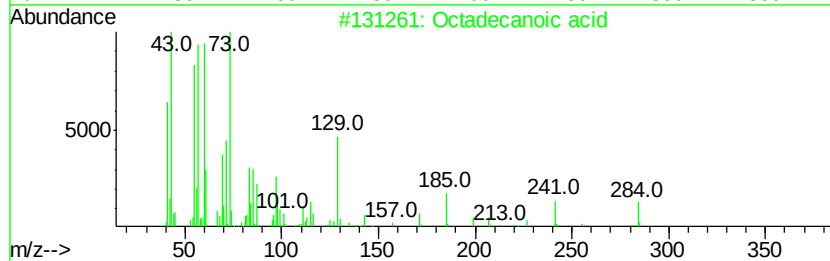
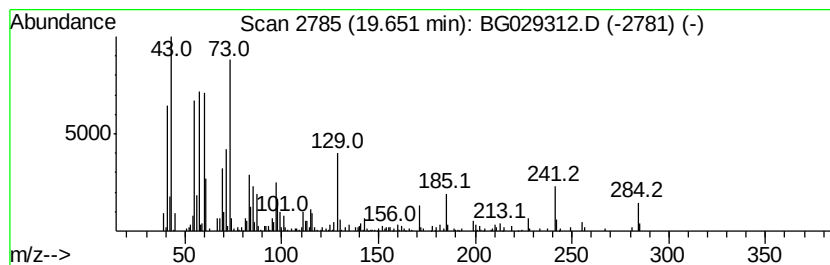
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.65	2.85 ng	195931	Phenanthrene-d10	17.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99	
2	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	87	
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74	
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64	
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64	



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101717\
Data File : BG029312.D
Acq On : 17 Oct 2017 22:11
Operator : SJ/JU
Sample : I5817-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	4.2	ng	95055	1	8.17	449667	20.0
unknown7.70	7.70	62.8	ng	1412120	1	8.17	449667	20.0
n-Hexadecanoic acid	18.39	2.0	ng	139986	4	17.52	1376540	20.0
Octadecanoic acid	19.65	2.9	ng	195931	4	17.52	1376540	20.0